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(FILE 'HOME' ENTERED AT 14:16:09 ON 10 FEB 2004)

FILE 'CA' ENTERED AT 14:16:30 ON 10 FEB 2004

L1 173937 S (POLYMER OR COPOLYMER OR POLYCARBONATE)AND(CATALY? OR (CONDENS? OR COCONDENS?)(6A)MELT?)
L2 2907 S L1 AND(SEARCH? OR SCREEN? OR DISCOVER? OR OPTIMI? OR ARRAY OR GRADIENT OR MULTIWELL OR MICROTIT?)
L3 2592 S L2 NOT(ENZYM? OR HYDROGENATION OR IMMUNO? OR DNA OR NANOTUBE)
L4 105 S L3 AND(POLYCARBONATE OR CARBONATE(2A)(POLYMER OR COPOLYMER) OR (MELT? OR SOLID STATE)(3A)(CONDENS? OR COCONDENS? OR POLYMERIZ? OR POLYMERIS?))
L5 8 S L3 AND(MULTIWELL OR MICROTIT? OR (ARRAY OR PLURAL?)(2A)WELLS)
L6 506 S L3 AND(SEARCH? OR SCREEN? OR DISCOVER? OR OPTIMI? OR GRADIENT)(4A) (CATALY? OR COMPOSITION OR MIXTURE OR MONOMER)
L7 451 S L6 NOT(FUEL CELL OR POLARONIC OR CATALY?(2A)(DECOMP? OR DEGRAD?))
L8 429 S L7 NOT(DISTILL? OR PAINT OR LOW TEMPERATURE)
L9 428 S L8 NOT(CARBON DIOXIDE(3A)MONOMER)
L10 359 S L9 NOT CROSSLINK?
L11 69 S L9 NOT L10
L12 3 S L11 AND POLYCARBONATE
L13 45 S L10 AND (HIGH THROUGHPUT OR CONBINATORIAL OR COMBINATORIAL)
L14 304 S L10 NOT(L13 OR LINKER OR PHOTO INDUC? OR PHOTOCATALY? OR PHOTO CATALY?)
L15 1 S L14 AND MATERIAL TRANSFORM?
L16 287 S L14 NOT L4-5,L15
L17 110 S L16 AND(COPOLYMER? OR CO POLYMER?)
L18 22 S L17 AND SYSTEM?
L19 177 S L4-5,L12-13,L15,L18

=> d bib,ab 1-177 119

L19 ANSWER 15 OF 177 CA COPYRIGHT 2004 ACS on STN

AN 139:27195 CA

TI Method for rapid **catalyst screening**

IN Lemmon, John Patrick

PA General Electric Company, USA

SO U.S. Pat. Appl. Publ., 7 pp.

PI US 2003119205 A1 20030626 US 2001-683416 20011224

PRAI US 2001-683416 20011224

AB The present invention provides methodol. for the rapid **discovery** of **catalytically-active** species. In the method of the invention, **gradient arrays** of **catalytic** species to be evaluated are absorbed on or impregnated into a support material. Next, the supported **array** is placed in a single reactor and the desired chem. reaction is carried out. The reaction products stream is then analyzed for the existence of the desired reaction products. If desired reaction products are obsd. to be present, the support library is divided at least in one half and the reaction conducted again. This technique is then repeated until a single **catalyst** mixt. (or multiple **catalyst** mixts.) is identified as having the desired **catalytic** activity.

L19 ANSWER 60 OF 177 CA COPYRIGHT 2004 ACS on STN

AN 136:357067 CA

TI Method for defining an experimental space and method and system for conducting **combinatorial high throughput screening** of **mixtures**

IN Cawse, James Norman; Wroczynski, Ronald James; Yang, Darchun Billy

PA General Electric Company, USA

SO PCT Int. Appl., 31 pp.

PI WO 2002035396 A1 20020502 WO 2001-US22222 20010713

PRAI US 2000-696071 A 20001025

AB A method comprises (A) defining a first exptl. space comprising factors of at least two mixts. with at least one common factor, (B) defining a second exptl. space by deleting duplicate factor combinations from the first exptl. space and (C) conducting an expt. on the second exptl. space. A system comprises a processor that (A) defines a first exptl. space

comprising factors of at least two mixts. with at least one common factor and (B) defines a second exptl. space by deleting duplicate factor combinations from the first exptl. space. The system also comprises a reactor and evaluator to select a best case set of factors from the second exptl. space by a **combinatorial high throughput screening** (CHTS) method to select a best case set of factors from the second exptl. space.

L19 ANSWER 61 OF 177 CA COPYRIGHT 2004 ACS on STN

AN 136:341185 CA

TI Method for **high-throughput** fluorescent **screening** of polymerization reactions

IN Potyrailo, Radislav Alexandrovich; May, Ralph Joseph; Shaffer, Robert Bentley; Lemmon, John Patrick; Wroczynski, Ronald James

PA General Electric Company, USA

SO PCT Int. Appl., 44 pp.

PI WO 2002033384 A1 20020425 WO 2001-US20246 20010626

US 6589788 B1 20030708 US 2000-690442 20001019

PRAI US 2000-690442 A 20001019

AB The present invention is directed to a method for the rapid **screening** of potential reactants, **catalysts**, and assocd. process conditions. In an embodiment, the invention comprises a method for evaluating **catalyst** efficacy in polymn. reactions (e.g., of **polycarbonates**) by the detn. of product mol. wt. and Fries products.

L19 ANSWER 79 OF 177 CA COPYRIGHT 2004 ACS on STN

AN 134:266737 CA

TI Method and apparatus for conducting **melt-polymerization** reactions

IN Warner, Gregory Lee; Flanagan, William Patrick; Lemmon, John Patrick; Potyrailo, Radislav Alexandrovich

PA General Electric Company, USA

SO PCT Int. Appl., 34 pp.

PI WO 2001021302 A1 20010329 WO 2000-US24537 20000908

PRAI US 1999-398679 A 19990920

AB In an exemplary embodiment, the app. includes a reaction vessel having an interior portion adapted to receive a reaction mixt. An agitator is disposed relative to the reaction vessel such that the agitator is capable of agitating the reaction mixt. A conduit is placed in fluid communication with the interior portion of the reaction vessel. A temp. probe is placed in thermal communication with the reaction vessel, and an optical analyzer adapted to perform real-time in situ anal. of the reaction mixt. is placed proximate or within the reaction vessel. In operation, the reaction is monitored and reaction conditions are adjusted, if necessary, to maintain the reaction within pre-detd. parameters. The reactor can be used for parallel **screening** of potential reactants and process conditions.

L19 ANSWER 80 OF 177 CA COPYRIGHT 2004 ACS on STN

AN 134:252754 CA

TI Testing **array** and method for small-scale evaluation of polymerization reactions in thin layers

IN Carnahan, James Claude; Lemmon, John Patrick; Potyrailo, Radislav Alexandrovich; Leib, Terry Kay; Warner, Gregory Lee

PA General Electric Company, USA

SO PCT Int. Appl., 35 pp.

PI WO 2001021301 A1 20010329 WO 2000-US24536 20000908

US 6307004 B1 20011023 US 1999-398677 19990920

PRAI US 1999-398677 A 19990920

AB A method for conducting parallel polymn. reactions in an **array** of reaction vessels, in which each reaction mixt. for each vessel comprises monomers embodied in a liq. such that the reactants form a film with a thickness sufficient to allow the polymn. rate to be essentially independent of mass transfer limitations. The reactions are then carried out, optionally in the presence of a **catalyst**, such that the homogeneity of the reaction mixt. is maintained without stirring. Such reactions (esp. for synthesis of **polycarbonates**, in which the reaction is driven by the volatility of a released byproduct) can be carried out on <50 mg reactant mixt. The method is useful for testing reactants, **catalysts**, and assocd. reaction parameters.

L19 ANSWER 85 OF 177 CA COPYRIGHT 2004 ACS on STN

AN 134:42537 CA

TI Solid phase thermal polymerization of macrocyclic bisphenol A carbonate tetramer using bisphenol A as initiator

AU Nagahata, Ritsuko; Sugiyama, Jun-Ichi; Goyal, Meenakshi; Asai, Michihiko; Ueda, Mitsuru; Takeuchi, Kazuhiko

CS Joint Research Center for Precision Polymerization-Tsukuba, Tsukuba, 305-8565, Japan

SO Polymer Journal (Tokyo) (2000), 32(10), 854-858

AB Solid phase thermal ring-opening polymn. of macrocyclic bisphenol A carbonate tetramer using bisphenol A as initiator was investigated. To find optimum conditions for the polymn., reactions were performed with various concns. of bisphenol A at different temps. and times. Under **optimized** conditions, colorless **polymer** with ultra high mol. wt. ($M_w > 1000000$) was produced in a short time. Terminal functionalities of the **polymers** were investigated with the help of matrix-assisted laser desorption ionization time-of-flight (MALDI-TOF) mass anal.

L19 ANSWER 88 OF 177 CA COPYRIGHT 2004 ACS on STN

AN 133:337145 CA

TI **High throughput** methodologies: a new paradigm for chemicals and materials research

AU Hewes, John D.

CS Technology Administration, National Institute of Standards and Technology, Advanced Technology Program, Chemistry and Life Sciences Office, U.S. Department of Commerce, Gaithersburg, MD, 20899-4730, USA

SO Chimica Oggi (2000), 18(9), 20-24

AB A new paradigm is now taking hold in the research and development (R&D) centers of Japanese, European, and U.S. advanced materials industries (**catalysts**, **polymers**, specialty and fine chems., optical materials, and electronic materials). **High throughput** methods for materials R&D are leveraging the **combinatorial** chem. methodologies developed over the past ten years in the pharmaceutical industry. The implementation of this emerging methodol. by materials innovators will enable new technologies having broad technol. and economic impact. The com. implication for **high throughput** methods will be more complex compns. created and analyzed in a reduced cycle time and at lower cost. The implication for basic research will be in elucidating new phenomena and in the development of new technol. platforms.

L19 ANSWER 92 OF 177 CA COPYRIGHT 2004 ACS on STN

AN 133:17925 CA

TI Melt polycondensation of L-lactic acid with Sn(II) **catalysts** activated by various proton acids: a direct manufacturing route to high molecular weight poly(L-lactic acid)

AU Moon, Sung Il; Lee, Chan Woo; Miyamoto, Masatoshi; Kimura, Yoshiharu

CS Department of Polymer Science and Engineering, Faculty of Textile Science, Kyoto Institute of Technology, Kyoto, 606-8585, Japan

SO Journal of Polymer Science, Part A: Polymer Chemistry (2000), 38(9), 1673-1679

AB Poly(L-lactic acid) (PLLA) was produced by the melt polycondensation of L-lactic acid. For the **optimization** of the reaction conditions, various **catalyst** systems were examd. at different temp. and reaction times. It was **discovered** that Sn(II) **catalysts** activated by various proton acids can produce high-mol.-wt. PLLA [wt.-av. mol. wt. (M_w) $\geq 100,000$] in a relatively short reaction time (≤ 15 h) compared with simple Sn(II)-based **catalysts** (SnO , $SnCl_2 \cdot 2H_2O$), which produce PLLA with an M_w of less than 30,000 after 20 h. The new **catalyst** system is also superior to the conventional systems in regard to racemization and discoloration of the resultant **polymer**.

L19 ANSWER 99 OF 177 CA COPYRIGHT 2004 ACS on STN

AN 131:351707 CA

TI Parallel solid-phase synthesis, **screening**, and encoding strategies for olefin-polymerization **catalysts**

AU Boussie, Thomas R.; Murphy, Vince; Hall, Keith A.; Coutard, Carla; Dales, Cameron; Petro, Miroslav; Carlson, Eric; Turner, Howard W.; Powers, Timothy S.

CS Symyx Technologies, Santa Clara, CA, 95051, USA

SO Tetrahedron (1999), 55(39), 11699-11710

AB A solid-phase protocol has been developed that allows for the parallel synthesis, **screening**, and chem. encoding of nickel (II) and palladium (II) olefin polymn. **catalysts**.

These **catalysts** display activity profiles comparable to the analogous homogeneous **catalyst** systems prep'd. by traditional methods. A chem. encoding strategy has also been developed which enables the chem. history of pooled solid-phase **catalysts** to be evaluated.

L19 ANSWER 101 OF 177 CA COPYRIGHT 2004 ACS on STN

AN 131:286019 CA

TI Parallel **combinatorial** approach to the **discovery** and **optimization** of **catalysts**, and uses thereof, for example in an enantioselective Strecker reaction

IN Jacobsen, Eric N.; Sigman, Matthew S.

PA President and Fellows of Harvard College, USA

SO PCT Int. Appl., 109 pp.

PI WO 9951546 A1 19991014 WO 1999-US7265 19990402

US 6316616 B1 20011113 US 1998-64462 19980422

PRAI US 1998-80461P P 19980402

AB The invention provides methods and compns., i.e. synthetic libraries of candidate compds., useful in the **discovery** and **optimization** of compds. which **catalyze** at least one chem. transformation. In certain instances, the subject compds. **catalyze** a chemoselective, regioselective, stereoselective, or enantioselective transformation. In particular, effective **catalysts** for the enantioselective addn. of HCN to imines (Strecker reaction) were designed through knowledge gained by 4 **combinatorial** libraries of sizes 12, 48, 132, and 70 compds. Thus, the **polymer**-supported tridentate Schiff base complex I [Sup = support; L1 and L2 = linkers; AA = amino acid; R, R', R'' = substituents; M = metal or 2 H atoms] was explored as a Strecker **catalyst**. The **catalysts** were prep'd. by sequential addn. of linker, amino acid, linker, diamine, and salicylaldehyde components. Application of library 1 (11 metals or bare ligand) to the addn. of t-BuSiMe₂CN to N-allylbenzalimine showed the unmetalated ligand (M = 2H) to be the most enantioselective (19% ee). Subsequent library members showed increased enantioselectivity due to several factors, including: (1) absence of L1; (2) use of Leu and even better, bulky L-amino acids such as Tle (tert-Leu) as the AA component; (3) use of thiourea as L2; (4) coupling of (R,R)-diamine components with use of L-amino acids; and (5) bulky substituents such as t-Bu on the salicylaldehyde-derived (phenolic) nucleus. Structural features leading to high enantioselectivity were unanticipated, with non-intuitive synergistic effects displayed between **catalyst** components. Based on the results, the unsupported **catalyst** II was designed. Use of this **catalyst** in a Strecker reaction of the imine t-BuCH:NCH₂Ph with HCN in PhMe at -78°, followed by workup with (CF₃CO)₂O, gave the trifluoroacetylated amino nitrile product (S)-t-BuCH(CN)N(CH₂Ph)COCF₃ in high yield with 95% ee. Using a similar combinatorially designed **catalyst**, the same imine starting material was used to synthesize tert-Leu in 65% overall yield and > 99% ee.

L19 ANSWER 120 OF 177 CA COPYRIGHT 2004 ACS on STN

AN 128:128586 CA

TI **Optimization** of olefin **copolymerization**. Effects of reaction parameters on **catalytic** activity and properties

AU Baumhardt-Neto, Ricardo; Galland, Griselda B.; Mauler, Raquel S.; Quijada, Raul

CS Instituto Quimica, Porto Alegre, 91501, Brazil

SO Polymer Bulletin (Berlin) (1998), 40(1), 103-109

AB The **copolymn.** of ethylene with 1-hexene using Et[Ind]₂ZrCl₂/MAO as **catalyst** was studied by multivariate methods. Three complete factorial designs were performed to study the influence of 1-hexene concn., reaction temp., and [Al]/[Zr] ratio on **catalytic** activity, **copolymer** viscosity, crystallinity, and m.p. Since the [Al]/[Zr] ratio has a small effect on the **catalytic** activity, a fourth design with 1-hexene and temp. was developed, giving higher **catalytic** activities. Temp. and 1-hexene concn. were the main effects found in the **system**. A second order effect arising from 1-hexene vs. [Al]/[Zr] ratio was also detected. **Polymer** viscosity, crystallinity, and m.ps. decreased with 1-hexene concn. Viscosity decreased with temp. whereas crystallinity increased when the temp. was raised from 30 to 60°.

L19 ANSWER 124 OF 177 CA COPYRIGHT 2004 ACS on STN

AN 127:109207 CA

TI Copolymerizations involving carbon dioxide: the use of CO₂ as a monomer

AU Super, Michael S.; Beckman, Eric J.

CS Bayer Corporation, New Martinsville, WV, 26155, USA

SO Trends in Polymer Science (Cambridge, United Kingdom) (1997), 5(7), 236-240

AB A review with 22 refs.; carbon dioxide is a relatively nontoxic, naturally abundant raw material whose use in high-value products has hardly been exploited. Unlike CO or SO₂, CO₂ cannot be copolymerized free radically, and will poison traditional transition-metal polymerization catalysts. Nevertheless, several researchers have shown that it can be copolymerized with other monomers to form polycarbonates, polyesters, polypyrones, polyurethanes and polyureas. The copolymerization of CO₂ has been extensively studied with in-depth looks at potential catalysts, possible comonomers and, lately, the possibility of using CO₂ as a solvent for its own copolymerization. The issues of catalyst activity, mechanism of reaction, appropriate solvents, copolymer molecular weight and polydispersity have all been examined, but a singular process that utilizes no organic solvent and produces a high weight-average molecular weight polymer (M_w > 50 000) with a low polydispersity (M_w/M_n < 1.3) from a highly active and well-defined catalyst remains to be discovered.

L19 ANSWER 130 OF 177 CA COPYRIGHT 2004 ACS on STN

AN 125:95787 CA

TI Synthesis and Characterization of Degradable Anhydride-co-imide Terpolymers Containing Trimellitylimido-L-tyrosine: Novel Polymers for Drug Delivery

AU Hanes, Justin; Chiba, Masatoshi; Langer, Robert

CS Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, MA, 02139, USA

SO Macromolecules (1996), 29(16), 5279-5287

AB The goal of this work is to synthesize a polymer specifically designed to deliver vaccine antigens. To accomplish this goal, a series of anhydride-co-imide terpolymers based on trimellitylimido-L-tyrosine (TMA-Tyr), sebacic acid (SA), and 1,3-bis(carboxyphenoxy)propane (CPP) was synthesized by melt condensation polymerization. It is desirable to incorporate tyrosine into the backbone of the polymer system due to its inherent ability to enhance the immune response to vaccine antigens. CPP and SA were copolymerized with the tyrosine derivative, TMA-Tyr, in order to develop a polymer with suitable material properties for drug delivery (e.g., high molecular weight, amorphous, and good solubility in low-boiling organic solvents), as well as to provide a series of polymers capable of a wide range of degradation and antigen release properties. To our knowledge, this paper represents the first report of the synthesis and characterization of terpolyanhydrides designed specifically to deliver drugs such as vaccine antigens. A systematic series of studies was performed to evaluate and optimize the influence of monomer ratio, reaction time and temperature, reaction catalysts, and catalyst concentration on polymer molecular weight, percent TMA-Tyr incorporation, and crystallinity. Terpolymers were synthesized with weight-average molecular weights in excess of 80 000 by using heterogeneous catalysts and highly purified monomers with low degrees of oligomerization. In addition, the terpolymers had no crystalline regions, the only exception being polymers with >60% SA in their backbone. Monomers and polymers were characterized by ¹H NMR and IR spectroscopy, elemental analysis, thermal transition temperature analysis, and gel permeation chromatography. The stability of these polymers in the solid state and in chloroform at various temperatures is also reported.

L19 ANSWER 155 OF 177 CA COPYRIGHT 2004 ACS on STN

AN 109:130664 CA

TI Acrylic copolymers with controlled properties

AU Sandescu, F.; Simionescu, C. I.

CS Ind. Cent. Synth. Fibers Yarns, Savinesti, Rom.

SO Angewandte Makromolekulare Chemie (1988), 161, 113-22

AB A method for control of copolymer endgroups in a solution-suspension copolymerization process was elaborated. The method was based on the utilization of an initiating system containing three components: S₂O₈²⁻/HSO₃⁻/Fe²⁺, their ratio and the ratio S₂O₈²⁻/comonomer mixture being optimized. In this way it was possible to control the content of endgroups of the copolymer, the saturation value, the number-average molecular weight values and polydispersity, without using comonomers with polar groups. Due to their conformational peculiarities and their packing manner in concentrated solutions, the macromolecular chains with a high endgroup content behaved much better during the solving and spinning processes. An increase in the content of copolymer endgroups favored not only the tinctorial properties, but also the spinnability of the spinning dopes obtained from the respective copolymers.

L19 ANSWER 159 OF 177 CA COPYRIGHT 2004 ACS on STN

AN 100:69006 CA

TI Polydispersity and scaling in linear **polymer** condensates

AU Daoud, M.; Family, F.

CS CEN-Saclay, Gif sur Yvette, 91191, Fr.

SO Journal de Physique (Paris) (1984), 45(1), 151-5

AB A linear **polymer** melt was considered where the chains were made by condensation of bifunctional monomers. In the very large distribution of mol. wts. that was obtained, typical and very large chains with different behaviors were distinguished. **Screening** was effective in the former, which acted as a (good) solvent for the latter. The cross-over mol. wt. (N^*) between the two classes was a function of the wt.-av. mol. wt. (N_w). Within a Flory approach, $N^* \sim N_w$ was found. Chains much larger than N^* were swollen. Typical chains had the same behavior in a monodispersed melt.

L19 ANSWER 163 OF 177 CA COPYRIGHT 2004 ACS on STN

AN 90:169037 CA

TI A new synthetic route to **polycarbonate**

AU Soga, K.; Hosoda, S.; Ikeda, S.

CS Res. Lab. Resour. Util., Tokyo Inst. Technol., Yokohama, Japan

SO Journal of Polymer Science, Polymer Chemistry Edition (1979), 17(2), 517-29

AB Metal carbonates were copolymd. with p-xylylene dihalides in the presence of crown ether **catalysts** to give poly(p-xylylene carbonate). Crown ethers having an 18-member ring showed the best **catalytic** activity of the various crown ethers investigated, and the polymn. was conducted in various solvents at 50-160° using 18-crown-6-ether (I) [17455-13-9]. Both the **polymer** yield and mol. wt. increased in proportion to the amt. of K_2CO_3 [584-08-7], and these increased rapidly and reached const. values with increasing concn. of I. The yield and mol. wt. also depended significantly upon the reaction temp. as well as the solvent used. A max. yield with the highest mol. wt. was obtained from the reaction at 100-200° in diglyme solvent. Spectroscopic anal. of the **polymers** indicated that all of the end groups had a benzyl bromide structure and, a plausible polymn. mechanism was proposed to explain these results. Similar polymns. were also conducted using several aliph. dibromides, $Br(CH_2)_nBr$, in place of p-xylylene dihalide. The products were strongly dependent on the value of n ; **polycarbonates** were obtained from dibromides having $n \geq 4$, while cyclic carbonates were obtained from dibromides having $n \leq 3$.

L19 ANSWER 176 OF 177 CA COPYRIGHT 2004 ACS on STN

AN 58:82287 CA

OREF 58:14174f-g

TI New polyoxamidation **catalysts**

AU Bruck, Stephen D.

CS E. I. du Pont de Nemours & Co., Inc., Wilmington, DE

SO Industrial & Engineering Chemistry Product Research and Development (1963), 2, 119-21

AB The usefulness of polyoxamide fibers for textile and industrial applications might be increased considerably if a process yielding spinnable products of higher mol. wts. were available. A series of new polyoxamidation **catalysts** belonging to Groups IVb and Vb was **discovered** that facilitate the prepn. of high-mol.-wt. polyoxamides with inherent viscosities of up to 1.54 (in m-cresol) by either solid-phase or **melt-phase polymerization**. Oxalic diesters can be treated with an appropriate diamine in the presence of As_2O_3 , Sb_2O_3 , SbF_3 , GeO_2 , Bi_2O_3 , or PbO to yield high-mol.-wt., spinnable **polymers**. The relative order of the effectiveness of these **catalysts** in promoting the polymerization process is: $SbF_3 \sim As_2O_3 \gg GeO_2 > Sb_2O_3 > Bi_2O_3 \sim PbO$.

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